BEC in a star-comb graph

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We investigate the properties of free bosons hopping on a star-comb network, discussing the single-particle spectrum and the main thermodynamic equilibrium properties: Bose-Einstein critical temperature, fraction of condensate, and spatial boson distribution. We find an enhancement of the critical temperature with respect to other inhomogeneous networks.

Although it is well known that free bosons hopping on translationally invariant networks cannot undergo Bose-Einstein condensation at finite temperature if the space dimension d is less or equal to two, very recent studies [1, 2, 3, 4] hint to the exciting possibility that the network topology may act as a catalyst for inducing a finite temperature spatial Bose-Einstein condensation even if d < 2. This is indeed possible if one resorts to a suitable discrete inhomogeneous ambient space on which bosons are defined. As an example of this situation we shall investigate the properties of non-interacting bosons hopping on a star-comb shaped network, evidencing that also in this case one may have a macroscopic occupation of the ground-state at low temperatures. Ultracold bosons in optical networks represent a physical system where this setup could be experimentally implemented.

The star-comb graph is a bundled graph which can be obtained by grafting a star graph to each site of a linear chain, called backbone (see Fig. 1). The sites of the graph can be naturally labelled introducing three integer indices (x,y,z) with $x,y,z\in Z$, where $x=1,\ldots,p$ labels the different arms on each star (excluding the links connecting the different stars), $y=0,\ldots,L$ represents the distance from the backbone and $z=1,\ldots,N_s$ labels the different stars. In the following we shall assume periodic boundary conditions $(x,y,1)\equiv (x,y,N_s+1)$. The Hamiltonian describing non-interacting bosons hopping on a star-comb graph can be written as:

$$H = -t \sum_{x,y,z; x',y',z'} A_{x,y,z; x',y',z'} \hat{a}_{x,y,z}^{\dagger} \hat{a}_{x',y',z'}.$$
 (1)

In Eq. (1), t is the hopping parameter while $\hat{a}_{x,y,z}^{\dagger}$ ($\hat{a}_{x,y,z}$) is the creation (annihilation) operator for bosons; $\hat{n}_{x,y,z} = \hat{a}_{x,y,z}^{\dagger}\hat{a}_{x,y,z}$ is the number operator at site (x,y,z). The filling, i.e., the average number of particles per site, is defined as $f = N_T/N_s(pL+1)$, where N_T is the total number of bosons and $N_s(pL+1)$ is the number of sites. The adjacency matrix of a star-comb graph is given by:

$$A_{x,y,z; x',y',z'} = (\delta_{y',y-1} + \delta_{y',y+1}) (1 - \delta_{y,0}) \delta_{x,x'} \delta_{z,z'} + \delta_{y,0} \delta_{y',1} \delta_{z,z'} + \delta_{y,0} \delta_{y',0} \delta_{x,x'} (\delta_{z',z-1} + \delta_{z',z+1}).$$
(2)

The eigenvalue equation $-t\sum_{j} A_{ij}\psi(j) = E\psi(i)$, with

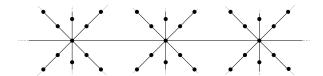


FIG. 1: The star-comb graph.

the previous labelling of sites, reads:

$$-t \sum_{x',y',z'} \left[(\delta_{y',y-1} + \delta_{y',y+1}) (1 - \delta_{y,0}) \delta_{x,x'} \delta_{z,z'} \right. \\ \left. + \delta_{y,0} \delta_{y',1} \delta_{z,z'} + \delta_{y,0} \delta_{y',0} \delta_{x,x'} (\delta_{z',z-1} + \delta_{z',z+1}) \right] \\ \cdot \psi(x',y',z') = E \psi(x,y,z)$$

$$(3)$$

By exploiting the translation invariance in the direction of the backbone, a Fourier transform in the variable z reduces Eq. (3) to a 1-dimensional eigenvalue problem. If one defines: $\psi(x,y,k) = \sum_z e^{ikz} \psi(x,y,z)$, with $k = 2\pi n/N_s$ and $n = 1, \ldots, N_s$, the eigenvalues equation (3) becomes:

$$-t \sum_{x',y'} \left[(\delta_{y',y-1} + \delta_{y',y+1}) (1 - \delta_{y,0}) \delta_{x,x'} + \delta_{y,0} \delta_{y',1} \right]$$

+
$$2\cos(k_0) \delta_{y,0} \delta_{y',0} \delta_{x,x'} \psi(x',y') = E\psi(x,y)$$
(4)

where $\psi(x,y,k) = \delta(k-k_0)\psi(x,y)$, with $k_0 = 2\pi n/N_s$, $n=0\ldots N_s$. Equation (4) can be regarded as the equivalent problem of a quantum particle hopping on a single star and interacting with a potential in the center, $V(k_0) = -2t\cos(k_0)$. The eigenvalues and eigenvectors of Eq. (4) are determined by requiring that the free particle solutions on the arms are solutions also in y=0. Indeed, for $y\neq 0$, the wave function satisfying Eq. (4) is:

$$\psi(x,y) = A_x e^{ihy} + B_x e^{-ihy} \tag{5}$$

Requiring that - on each arm - $\psi(x,y)$ is a solution of the eigenvalue equation at y=L introduces restrictions on the parameters h, A_x , B_x , and on the eigenvalues E. In other words, it amounts to require that A_x , B_x and h should satisfy the p equations

$$-t\left(A_x e^{ih(L-1)} + B_x e^{-ih(L-1)}\right)$$

$$= -2t\cos(h)\left(A_x e^{ihL} + B_x e^{-ihL}\right)$$

$$x = 1, \dots, p.$$
(6)

The eigenstates defined in Eq. (5) should also satisfy (p-1) matching conditions in the center of each star. Thus, one has

$$A_x + B_x = A_{x+1} + B_{x+1}$$
 $x = 1, \dots, p-1.$ (7)

Using Eqs. (7), the condition in one of the centers gives one more equation

$$-t \left[\sum_{x=1}^{p} \left(A_x e^{ih} + B_x e^{-ih} \right) + 2\cos(k_0) \left(A_x + B_x \right) \right]$$

$$= -2t \cos(h) \left(A_{x'} + B_{x'} \right),$$
(8)

with $x = 1, \dots, p$. Equations (6) and (8) may be grouped in a homogeneous linear system of 2p equations which allows to fix the 2p parameters A_x and B_x . Upon denoting with Q the $(2p \times 2p)$ matrix whose elements are the coefficients of the linear system given by Eqs. (6) and (8), and requiring that

$$\det Q = \Theta(h, L)(1 - e^{2ih(L+1)})^{p-1} \cdot \{(p-2)\cos(h) - p\cot[h(L+1)]\sin(h) + 2\cos(k_0)\}$$
(9)

is equal to zero, the solution is unique. In Eq. (9) $|\Theta(h,L)| = 1$ for any value of h.

One immediately sees that the values of h for which $h = n\pi/(L+1)$ (with n = 1, 2, ..., L) provide a set of L(p-1)-fold degenerate eigenstates of Eq. (9) for each value of k_0 (in total N_s sets). In addition, the solutions of the transcendental equation

$$(p-2)\cos(h) - p\cot[h(L+1)]\sin(h) + 2\cos(k_0) = 0$$
(10)

provide the values of h associated to non-degenerate eigenstates. Equation (10) can be solved numerically and yields a set of $N_s(L-1)$ non-degenerate eigenvalues corresponding to different values of k_0 and to values of h which - in the thermodynamic limit - are equally spaced and separated by a distance $\pi/(L+1)$. As a result, each set of delocalized states is formed by (pL-1) states corresponding to energies ranging between -2t and +2t. If the potential in the center $V(k_0)$ is equal to zero, one recovers the same condition of the single star [4].

Since the total number of states should equal $N_s(pL+1)$, there are still $2N_s$ localized states in the spectrum. These states belong to the so-called hidden spectrum [1]. To find them, it is convenient to look for solutions of the eigenvalue equation (3) of the form

$$\psi_{-}(y) = Ae^{-\eta y} + Be^{\eta y}$$

$$\psi_{+}(y) = A(-1)^{y}e^{-\eta y} + B(-1)^{y}e^{\eta y},$$
(11)

corresponding, respectively, to the eigenvalues of the lower hidden spectrum $\sigma_{-} = -2t \cosh \eta$ and to the eigenvalues of the upper hidden spectrum $\sigma_{+} = 2t \cosh \eta$. In Eqs. (11), A and B are normalization constants and $\eta \equiv 1/\xi$ is a parameter accounting for the localization of the states. By rewriting Eq. (10) for $h = i\eta$, one has to solve:

 $(p-2)\cosh(\eta) - p \coth\left[\eta(L+1)\right] \sinh\left(\eta\right) + 2\cos(k_0) = 0, \tag{12}$ together with the condition that $\sum_{x,y} |\psi_0(x,y)|^2 = 1$. In the thermodynamic limit, $L \to \infty$, Eq. (12) becomes: $(p-2)\cosh(\eta) - p \sinh\left(\eta\right) + 2\cos(k_0) = 0$, which is solved by $\eta = \log\left[p-1+2\cos k_0(p-1+\cos^2 k_0)+2\cos^2 k_0\right]$, yielding, for the lower hidden spectrum: $\sigma_- = -t\left[(p-2)\cos(k_0)+p\sqrt{p-1+\cos^2(k_0)}\right]/(p-1)$. The lowest energy level is obtained for $\cos(k_0) = 1$; one has

$$E_0 = -t \frac{(p-2) + p\sqrt{p}}{p-1}. (13)$$

Solving the eigenvalue equation (3) for $E = E_0$, one obtains the wavefunction of the localized ground-state:

$$\psi_{E_0}(y) = \sqrt{\frac{\sqrt{p} + 2}{2(\sqrt{p} + 1)}} e^{-y/\xi}.$$
 (14)

 $\xi = 1/\log(\sqrt{p}+1)$ provides an estimate of the groundstate localization. The ground state is localized along the backbone and it decreases exponentially along the arms. When p = 2, one immediately recovers all the known results of the comb graph [1, 3]. For each value of k_0 $(\cos(k_0) > 0)$ there is a solution of (12) with a different energy in the interval $[E_0, -2t]$. In a finite star-comb with $N_s(pL+1)$ sites there are N_s solution of this type and for $N_s \to \infty$ these solutions fill densely the interval $[E_0, -2t]$. Analogously, when $\cos(k_0) < 0$ there are N_s solution of (12) corresponding to the spectral region at high energy $(E = [2t, |E_0|])$, where the other hidden states appear. In Fig. 2a we plot the ground-state wavefunction for p = 10 for a single star (dashed line) and for a star-comb (solid line) as a function of the distance from the backbone. Figure 2a evidences that adding stars enhances the localization of the wavefunction around the center of each star.

The thermodynamic properties of non-interacting bosons hopping on a star-comb graph evidence also in this case a topology induced spatial BEC even if d < 2 [1, 2]. To elucidate this phenomenon, it is most convenient to introduce the macrocanonical ensemble to determine the fugacity $z = e^{\beta(\mu - E_0)}$ as a function of the temperature [1]: the equation determining z is given by

$$N_T = \sum_{E \in \sigma} \frac{d(E)}{z^{-1} e^{\beta(E - E_0)} - 1}.$$
 (15)

In Eq. (15), d(E) is the degeneracy of each single-particle eigenstate of the Hamiltonian (1) and $\beta = 1/k_BT$. The

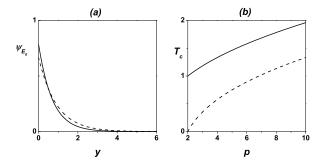


FIG. 2: (a) The normalized single-particle ground-state wavefunction for bosons hopping on a star and star-comb graphs as a function of the distance y from the center. The number of arms is p=10. (b) Critical temperature T_c (in units of k_B/E_J) as a function of the number of arms p. The solid lines are for the star-comb graph, whereas the dashed lines are for the single star.

sum in Eq. (15) is over the entire spectrum σ . For free bosons hopping on a star-comb graph, one has

$$N_{T} = N_{E_{0}}(L, T) + N_{\sigma_{-}}(L, T) + N_{\sigma_{+}}(L, T) + \int_{E \in \sigma_{0}} dE \, \frac{N_{s}(pL+1)\rho(E)}{z^{-1}e^{\beta(E-E_{0})} - 1},$$
(16)

where $N_{E_0}(L,T)$, $N_{\sigma_-}(L,T)$ and $N_{\sigma_+}(L,T)$ denote, respectively, the number of particles at a certain temperature T in the ground-state and in the two regions σ_- and σ_+ of the hidden spectrum. $\rho(E)$, with $E \in \sigma_0$, is the energy density of states of the linear chain, i.e., $\rho = 1/(\pi\sqrt{4t^2 - E^2})$, with σ_0 being the region of the spectrum corresponding to delocalized states. The last term of the right-hand side of Eq. (16) is the number of bosons in the delocalized (chain-like) states. The presence of the hidden spectrum changes the behavior of the integral evaluated in the interval $\{-2t, 2t\}$, since it reduces it to the one describing non-interacting bosons on a linear chain with an impurity in one of the sites. As a result, letting $z \to 1$, the integral converges even at finite temperatures making possible a spatial BEC in d < 2.

If one defines T_c as the critical temperature at which BEC occurs, then for any $T < T_c$ the ground-state is macroscopically filled. Since, at the critical temperature, $N_{E_0}(T_c) = N_{\sigma_{\pm}}(T_c) = 0$, the equation allowing to determine T_c as a function of the parameters f and t reads:

$$\pi f = \int_{-2t}^{2t} \frac{dE}{\sqrt{4t^2 - E^2}} \frac{1}{e^{(E - E_0)/(k_B T_c)} - 1}.$$
 (17)

Equation (17) can be solved numerically for any value of f. When $f \gg 1$, one may expand the exponential in Eq. (17) to the first order in the inverse of the critical temperature T_c . Upon inserting the value of the ground-state energy (13) in Eq. (17), one easily finds that the

critical temperature T_c is given by

$$T_c \approx \frac{tf}{k_B} \frac{\sqrt{p} \left(2 + \sqrt{p}\right)}{1 + \sqrt{p}}.$$
 (18)

Equation (18) has been checked numerically and it is in excellent agreement with the numerical solution of Eq. (17) for $f \gg 1$, the error being of order 1/f. If one compares the critical temperature of the single star and of the star-comb graphs, one immediately sees that, once the number of arms is fixed, T_c is always enhanced in the latter realization. This is shown in Fig. 2b.

One may now use Eq. (18) to determine the condensate fraction as a function of the scaled temperature T/T_c . In the thermodynamic limit, the number of particles in the delocalized states is given by

$$N_{\sigma_0} = \lim_{L \to \infty} N_s(pL+1) \int_{E \in \sigma_0} \rho(E) \frac{dE}{e^{\beta(E-E_0)} - 1}$$

$$\approx N_T \frac{T}{T_c}.$$
(19)

In the last equation the exponential has been expanded to the first order in β : this approximation holds for $f \gg 1$ and it is in very good agreement with the numerical evaluation of the integral in Eq. (19) also in a large neighborhood below T_c . From Eqs. (16) and (19) one gets the number of particles in the localized states $N_0 = N_{E_0} + N_{\sigma_-}$: the fraction of condensate, for $T < T_c$, is then given by

$$\frac{N_0}{N_T} \approx 1 - \frac{T}{T_c}. (20)$$

For f ranging from 10^3 to 10^9 , the results provided by Eq. (20) differ from those obtained by the numerical evaluation of N_0 from Eq. (16) by less than 1%. Equation (20) clearly shows that the condensate has dimension 1 just as cigar-shaped one-dimensional atomic Bose condensates [5].

Due to the topology induced spatial condensation on the backbone, one should expect an inhomogeneous distribution of the bosons along the arms of the network. The average number of bosons N_B at a site (x,y,z) depends - due to the symmetry of the graph - only on the distance y from the backbone. It is not difficult to show (see also Ref. [3]) that, away from the backbone $(y\gg 1)$ and once the filling is fixed, N_B depends only on the scaled temperature T/T_c and it is given by

$$\frac{N_B(y; T/T_c)}{f} \approx \frac{T}{T_c}. (21)$$

Topology induced spatial BEC in a system of noninteracting bosons hopping on a star-comb graph predicts then a rather sharp decrease of the number of bosons at sites located away from the backbone. The linear dependence is consistent with the observation that, in this system, the condensate has dimension 1. In this paper we have investigated in detail another situation where the role played by the network's topology is crucial in determining the thermodynamic properties of the system. We focused on the properties of free bosons hopping on a star-comb network, finding an enhancement - with respect to other inhomogeneous structures previously investigated $[1,\,2,\,3,\,4]$ - of the critical temperature at which the particles condense.

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